An Adjoint Approach for the Estimation of Source Terms for Atmospheric Releases

23 February, 2012

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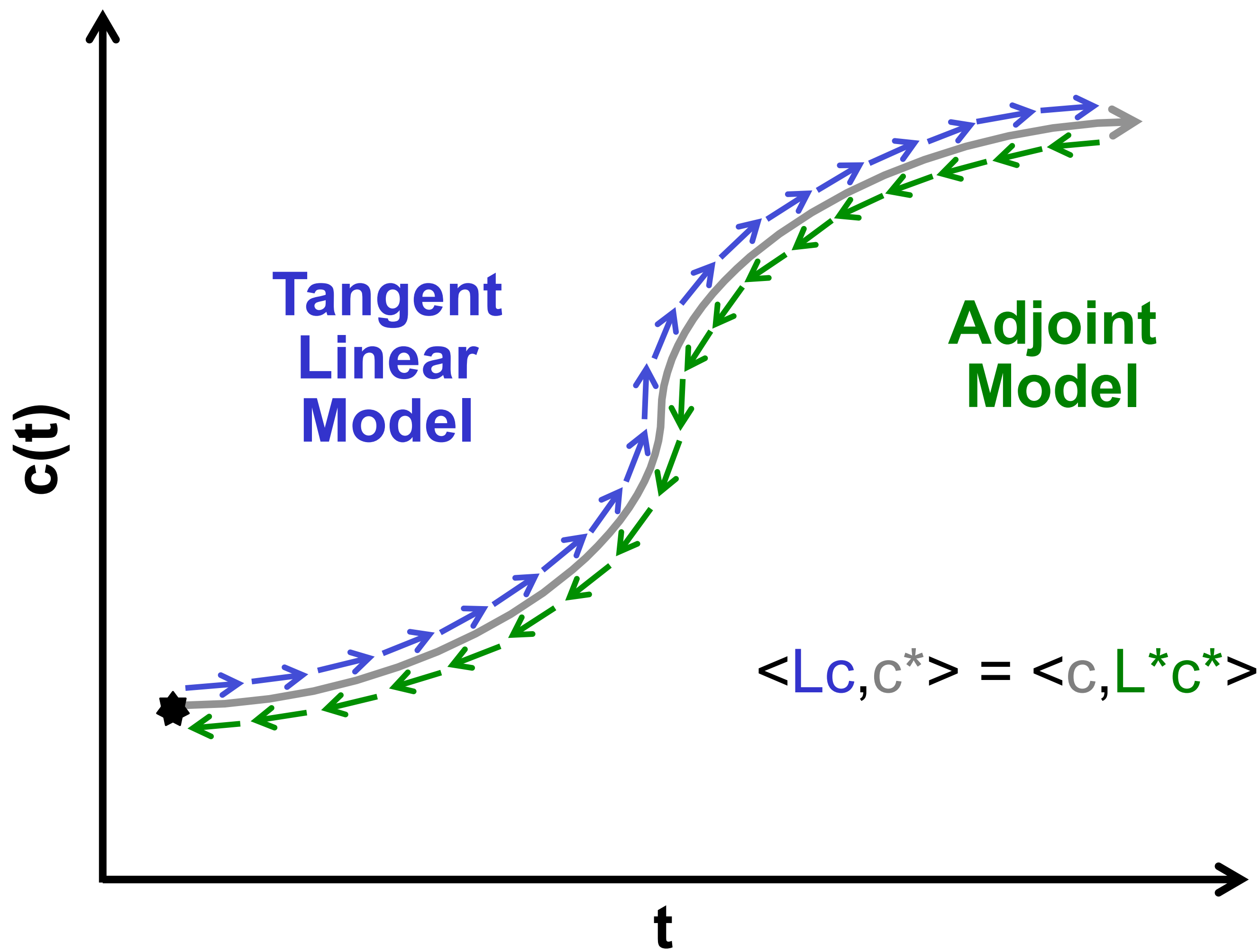
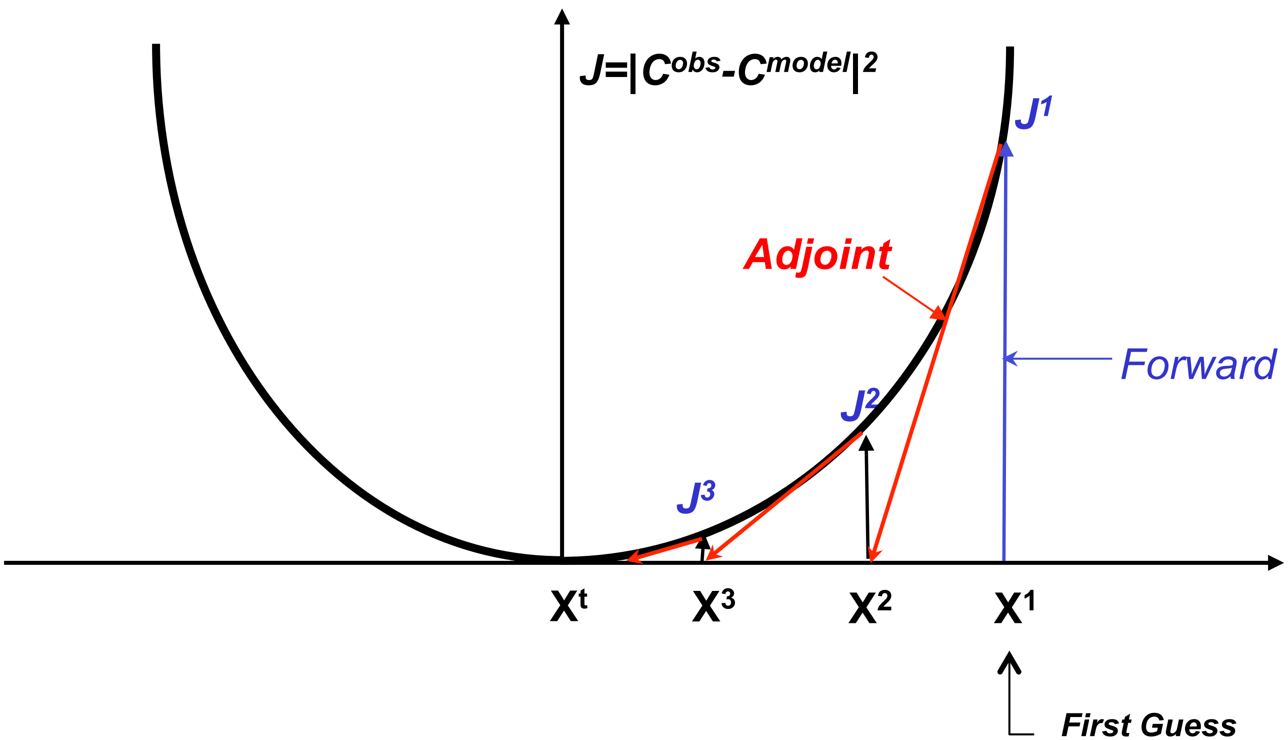
National Center for Atmospheric Research

Adjoint



Gradient Descent Minimization



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Outline

- **Chemical, Biological, Radioactive, or Nuclear (CBRN) Source Term Estimation (STE) examples**
  - **High quality meteorological data**
  - **Poor quality meteorological data**
- **Utilizing information on uncertainty in observations**
  - **Cost function visualization and scaling**
  - **STE variable uncertainty relations**
- **Uncertainty mapping**
  - **Physics-based method (uncertainty are inputs to constrain adjoint)**
  - **Ensemble-based method (adjoint to define the initial uncertainty)**

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Operational Chemical, Biological, Radiological, and Nuclear (CBRN) Defense Problem

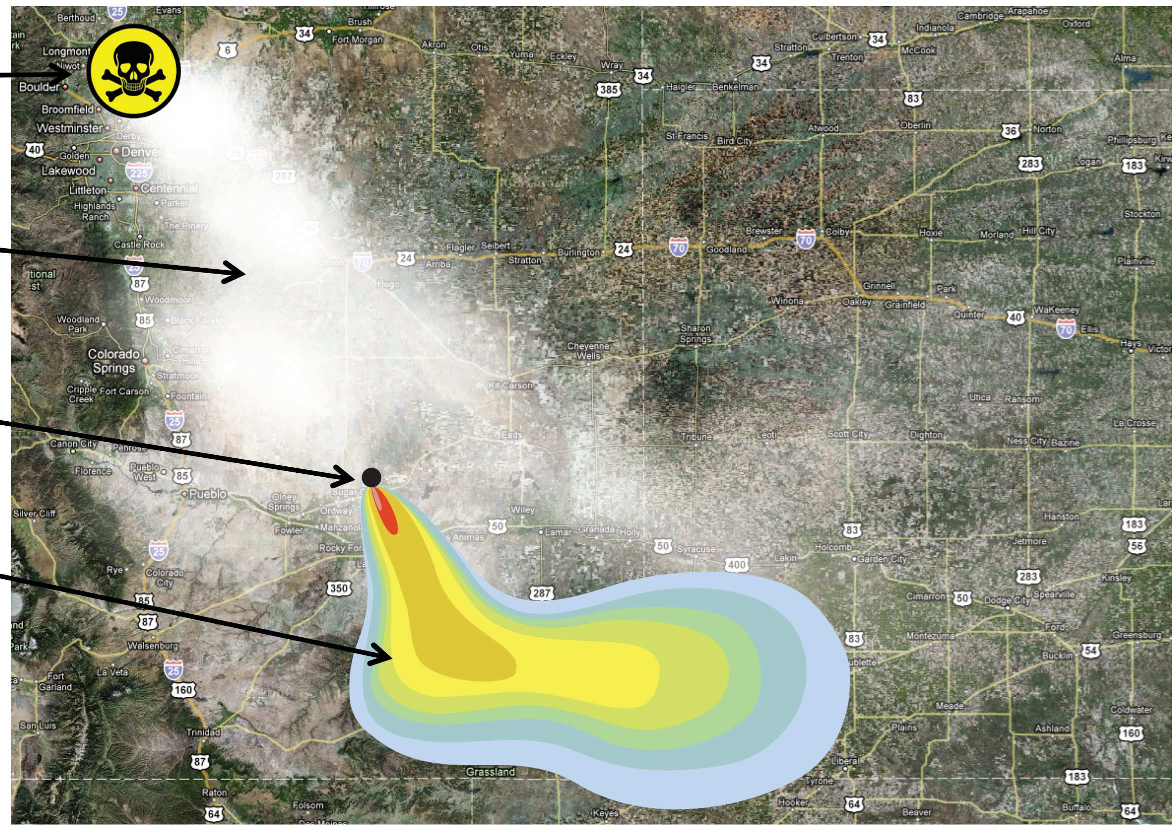
- **Scenario**
  - A sensor or sensor network detects CBRN materials
  - Detection is currently used as the source to forecast the downwind impact
  - The initial forecast may not accurately reflect the actual threat

Actual Release Location

Actual CBRN Plume

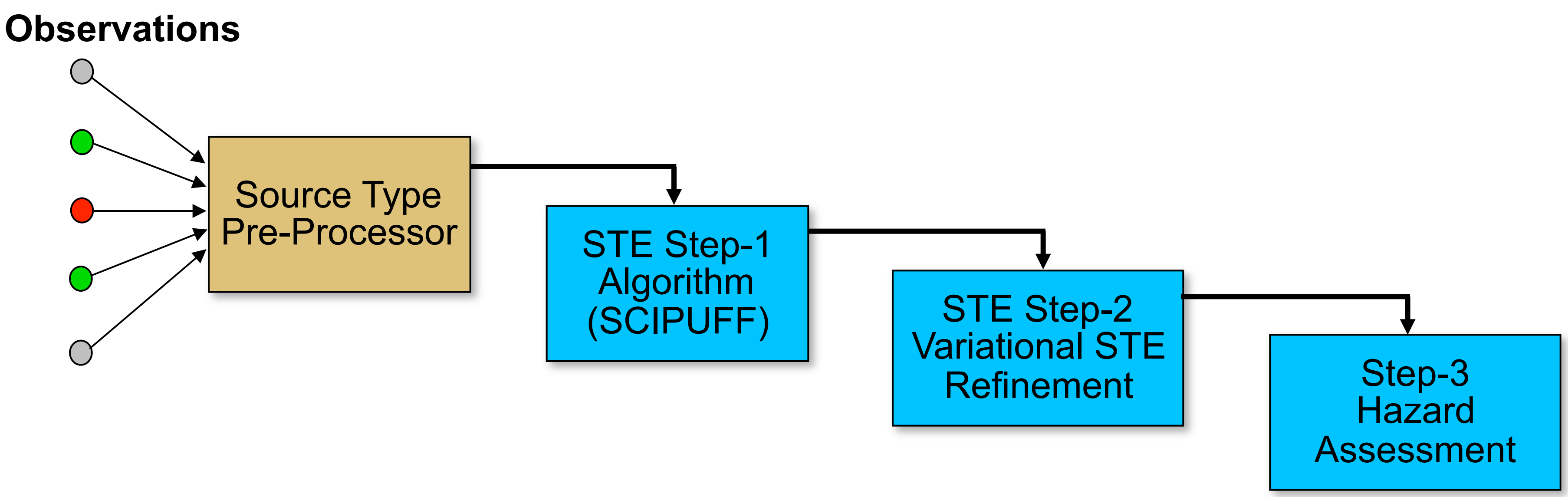
CBRN Sensor Location

Sensor Detection Based Plume



High Level
CBRN STE Algorithm Design

- **STE algorithm design constraints**
  - **Ability to utilize varying types and frequency of observations**
  - **Compatible with Second-order Closure Integrated PUFF (SCIPUFF) and Joint Effects Model (JEM) system designs**
  - **Suitable to run on a laptop (e.g. computationally efficient)**
  - **Answer available within seconds to minutes of starting the STE job**



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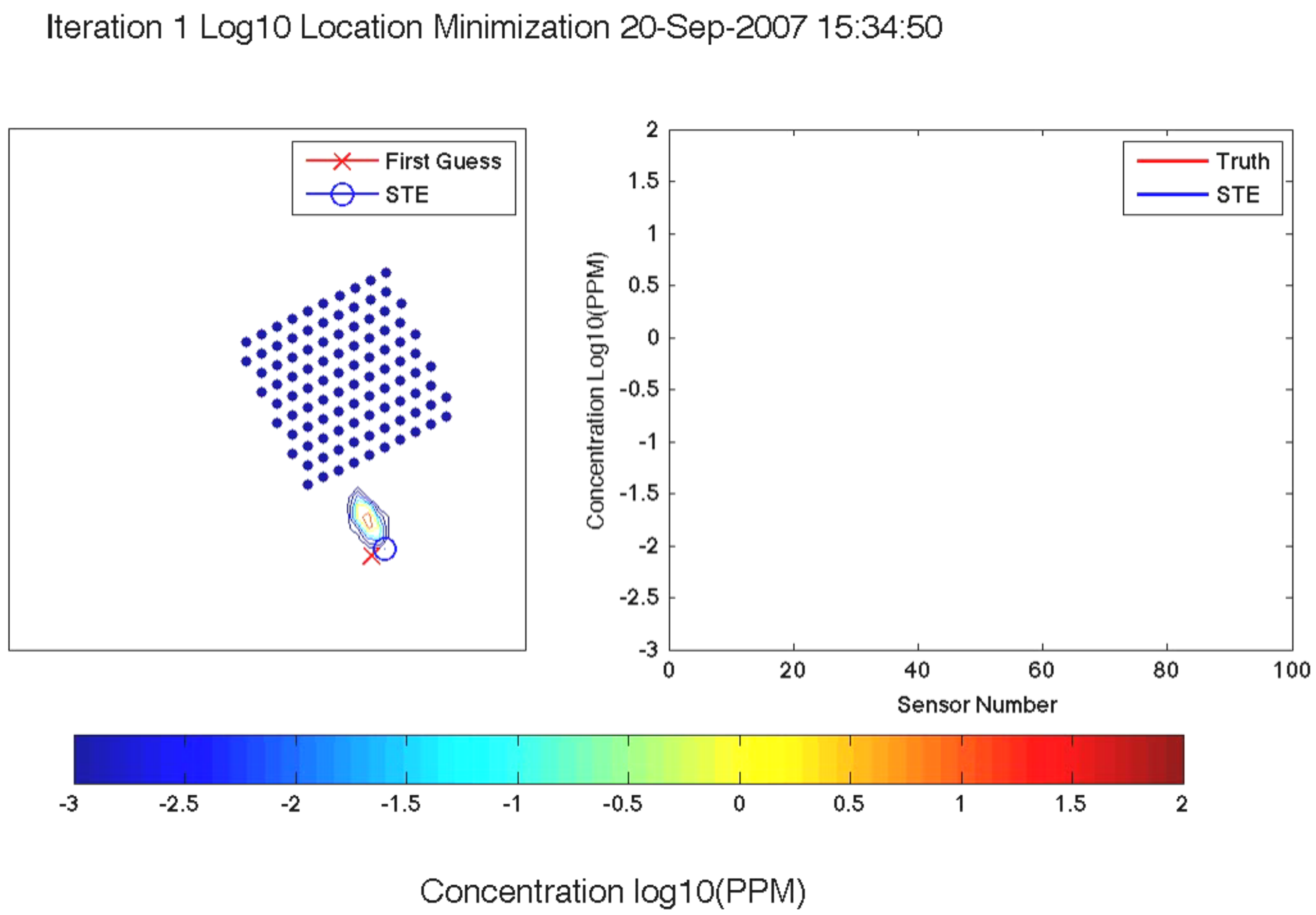
STE Algorithm Example



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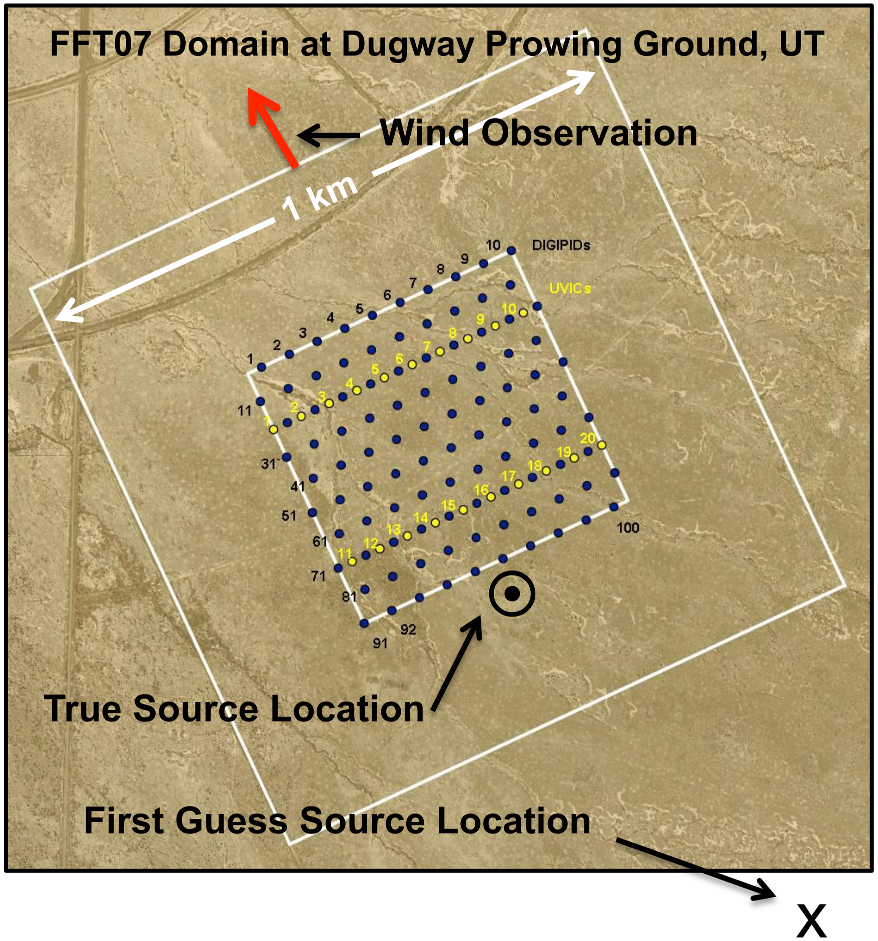
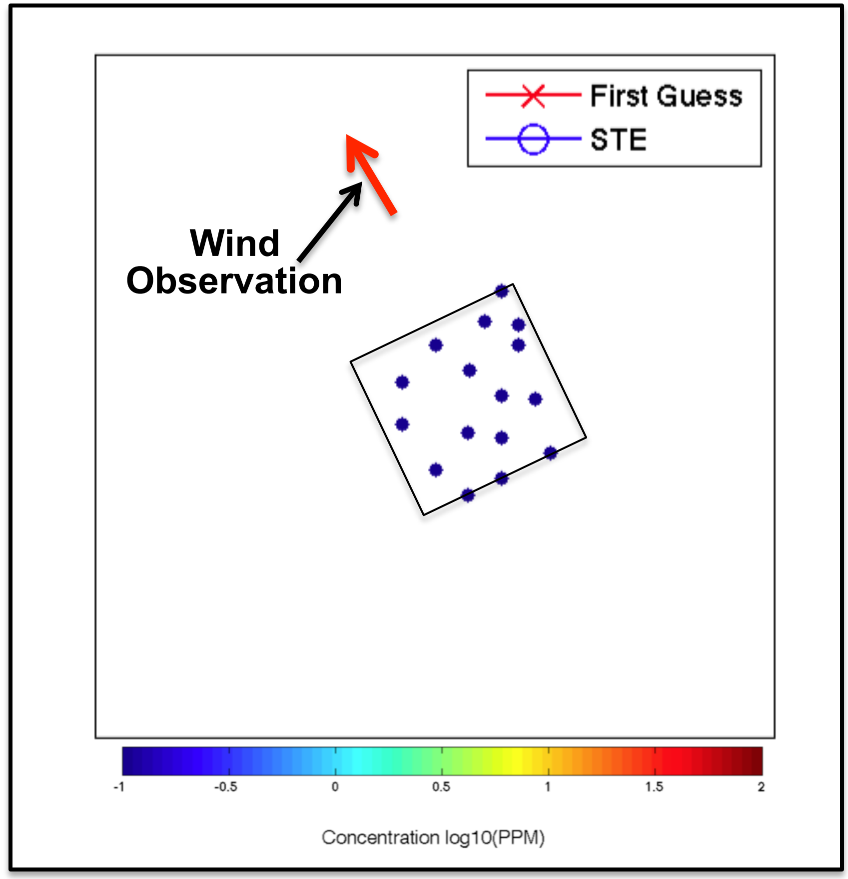
Wind Adjustment in CB STE Algorithm

(FFT07* Case 61)





***FUsing Sensor Integrated Observing Network (FUSION) Field Trials 2007 (FFT07)**

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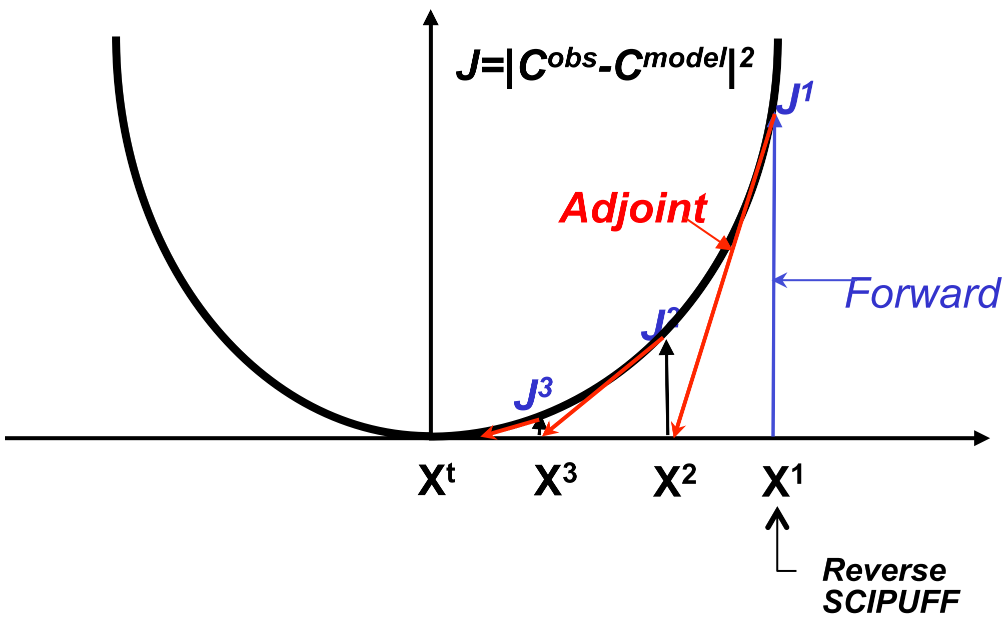
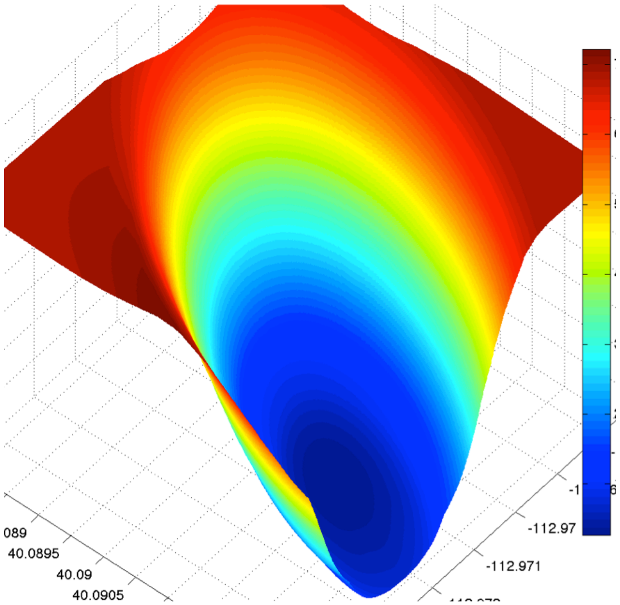
Cost Function Visualization

Schematic of Cost



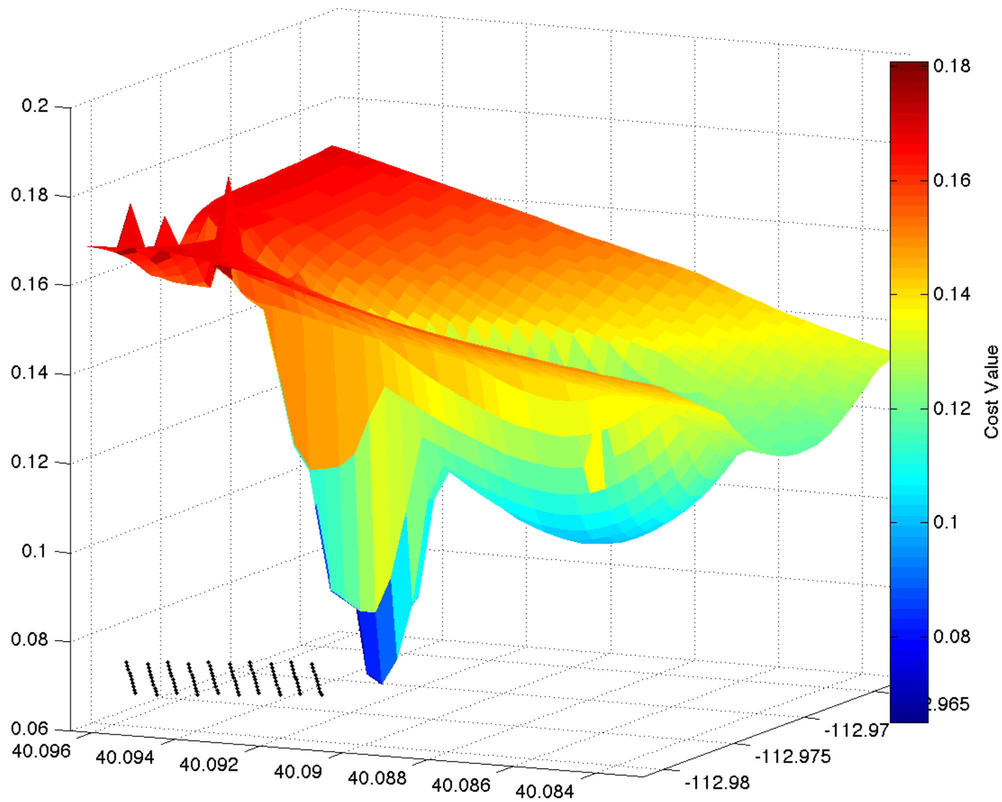
Cost Surface for Location



Cost Function and Uncertainty

Emission rate	Along wind source location	Cross wind source location	Source height	Time of release	Wind Speed	Wind Direction	Concentration observations

$$2J = \left[\frac{q_s^{bck} - q_s}{\sigma^q}\right]^2 + \left[\frac{x_s^{bck} - x_s}{\sigma^x}\right]^2 + \left[\frac{y_s^{bck} - y_s}{\sigma^y}\right]^2 + \left[\frac{z_s^{bck} - z_s}{\sigma^z}\right]^2 + \left[\frac{t_r^{bck} - t_r}{\sigma^t}\right]^2 + \left[\frac{U_e^{bck} - U_e}{\sigma^U}\right]^2 + \left[\frac{\theta_e^{bck} - \theta_e}{\sigma^\theta}\right]^2 + \left[\frac{C^{obs}(t) - C(t)}{\sigma^{obs}}\right]^2$$



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Ambiguity in STE variables

(Plume Reference Frame)

X_p Y_p

T Q

U θ

X_p [m] ⇔ U [m/s] ⇔ Q [kg/s]

X_p [m] ⇔ U [m/s] ⇔ T [s]

X_p [m] ⇔ T [s] ⇔ Q [kg/s]

Y_p [m] ⇔ θ [°]

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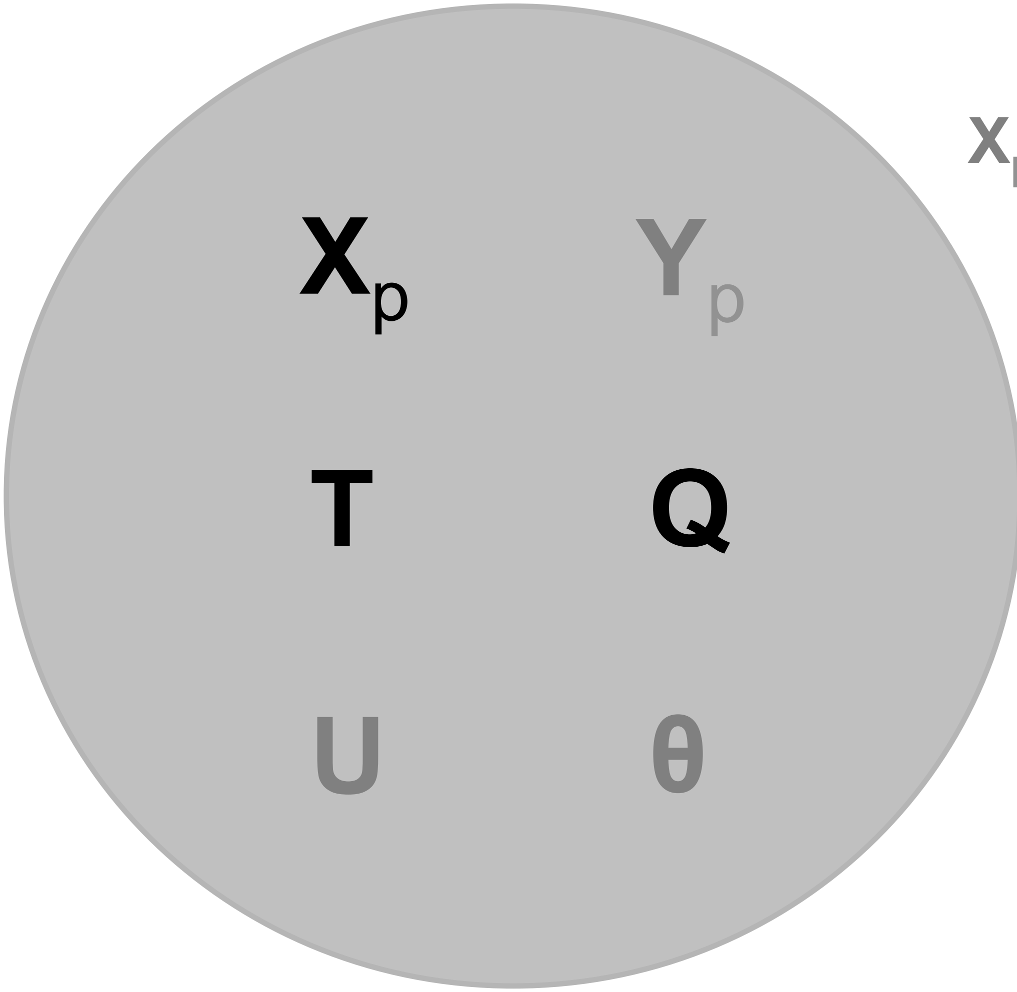

X_p [m] $\Leftrightarrow$ U [m/s] $\Leftrightarrow$ Q [kg/s]

X_p [m] $\Leftrightarrow$ U [m/s] $\Leftrightarrow$ T [s]

X_p [m] $\Leftrightarrow$ T [s] $\Leftrightarrow$ Q [kg/s]

Y_p [m] $\Leftrightarrow$ θ [°]

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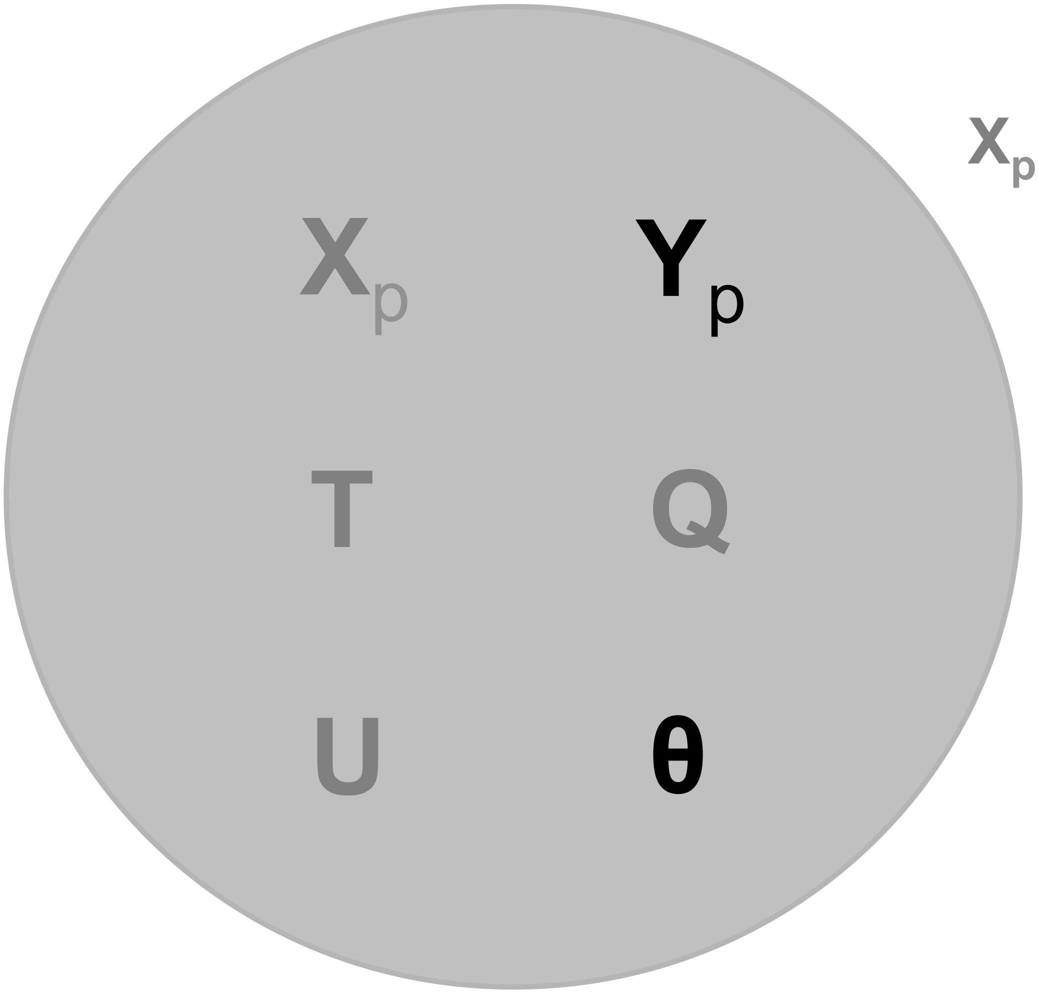

X_p [m] ⇔ U [m/s] ⇔ Q [kg/s]

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Cost Function
(Uncertainty Mapping)

The Cost Function is defined as:

$$J = \left(\frac{1}{2}[C^{obs}(t) - C(t)]^T [R]^{-1} [C^{obs}(t) - C(t)]\right) + \left(\frac{1}{2}[A_m]^T [E_B]^{-1} [A_m]\right)$$

Current definition of Background Error Covariance Matrix (E_B) used:

$$E_B = \begin{bmatrix} \sigma^2_{STE\,1} & 0 & 0 & 0 \\ 0 & \sigma^2_{STE\,2} & 0 & 0 \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \sigma^2_{STE\,n} \end{bmatrix}$$

Full Background Error Covariance Matrix (E_B):

$$E_B = \begin{bmatrix} \sigma^2_{xx} & cov(x,y) & cov(x,z) & cov(x,q) & cov(x,U) & cov(x,\theta) & cov(x,t) \\ cov(y,x) & \sigma^2_{yy} & cov(y,z) & cov(y,q) & cov(y,U) & cov(y,\theta) & cov(y,t) \\ cov(z,x) & cov(z,y) & \sigma^2_{zz} & cov(Z,q) & cov(z,U) & cov(z,\theta) & cov(z,t) \\ cov(q,x) & cov(q,y) & cov(q,z) & \sigma^2_{qq} & cov(q,U) & cov(q,\theta) & cov(q,t) \\ cov(U,x) & cov(U,y) & cov(U,z) & cov(U,q) & \sigma^2_{UU} & cov(U,\theta) & cov(U,t) \\ cov(\theta,x) & cov(\theta,y) & cov(\theta,z) & cov(\theta,q) & cov(\theta,U) & \sigma^2_{\theta\theta} & cov(\theta,t) \\ cov(t,x) & cov(t,y) & cov(t,z) & cov(t,q) & cov(t,U) & cov(t,\theta) & \sigma^2_{tt} \end{bmatrix}$$

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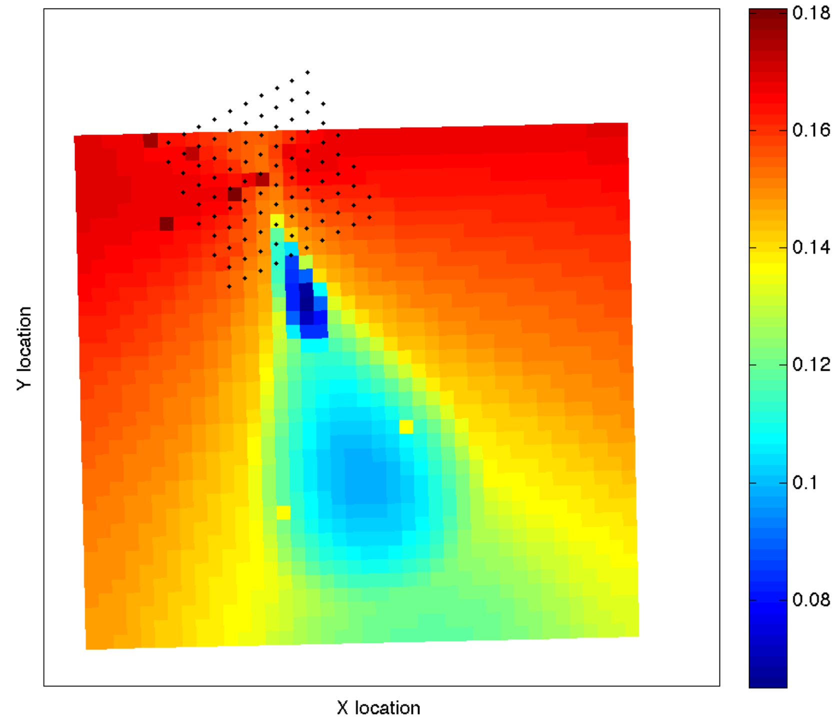
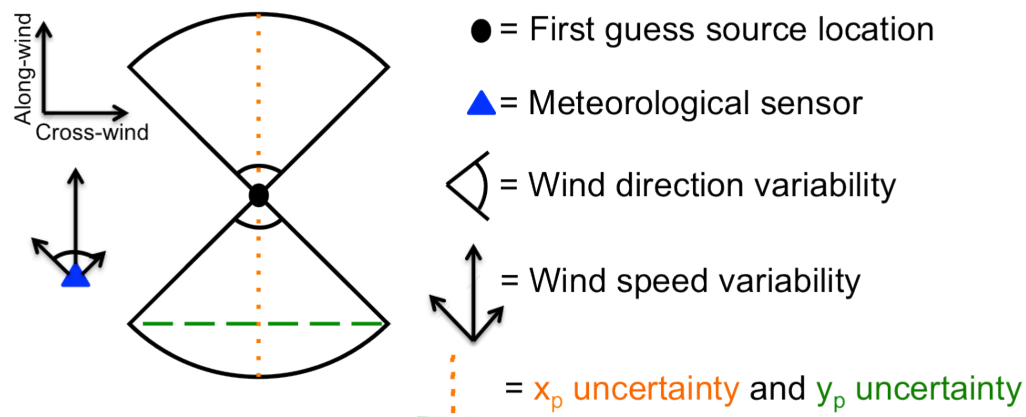
Background Error Covariance Matrix

(Instantaneous Release Example)

2D Visualization



Physics-Based Method



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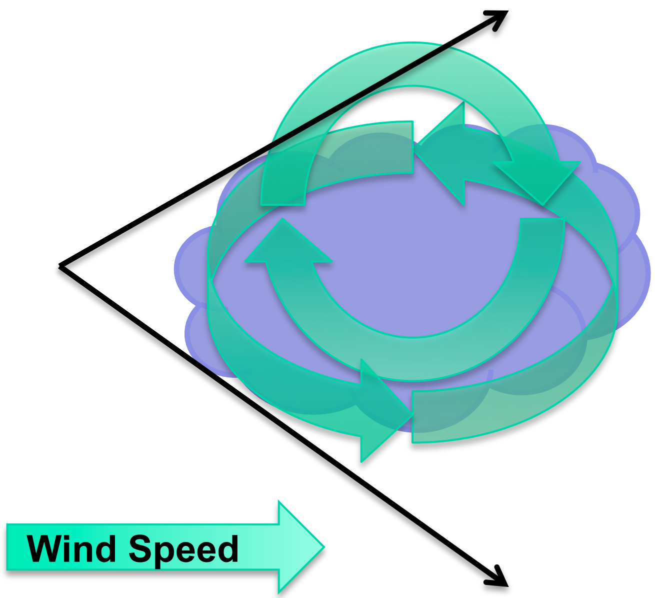
Exploiting Uncertainty Relationships

(Meteorological Uncertainty)

- **Use wind variability to constrain location**
  - Trend
  - Plume meander
  - Plume diffusion

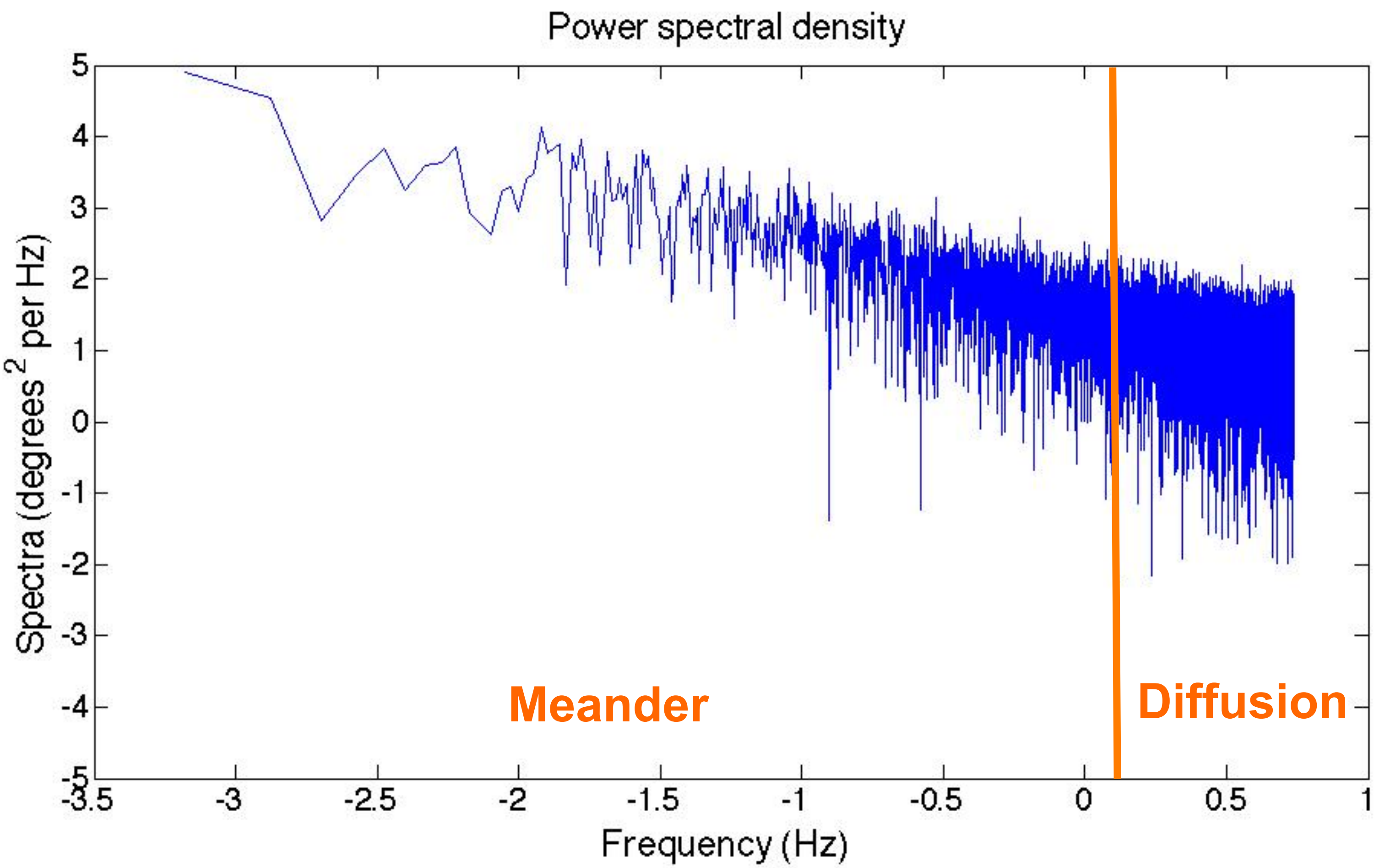
- **Can we filter the winds to distinguish the meander and diffusion?**



$$\text{Eddy time scale} = \frac{\text{Mean wind speed}}{\text{Width of plume}}$$

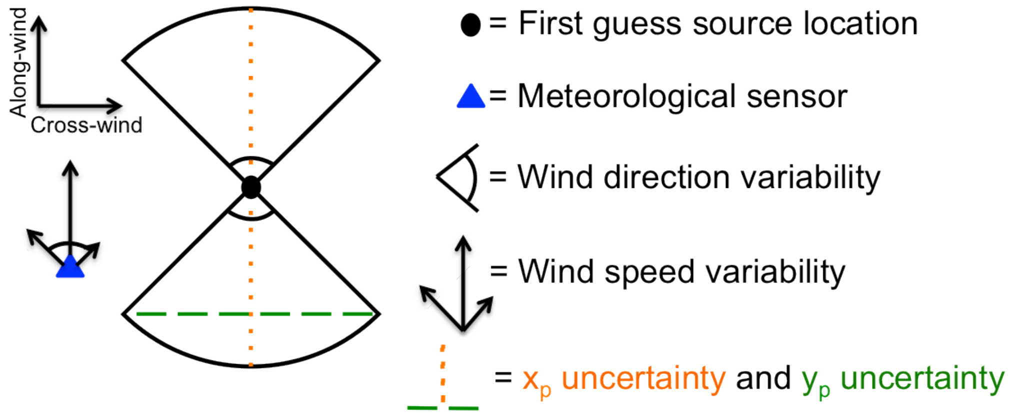
Deriving Wind Direction Uncertainty

(FFT07 Trial 54)



Eddy time scale = $\frac{\text{Mean wind speed}}{\text{Width of plume}}$ = Cutoff Frequency

Inversion and Scaling



$$\sigma_{xx} = \sigma_{UU} \times \sigma_{tt},$$

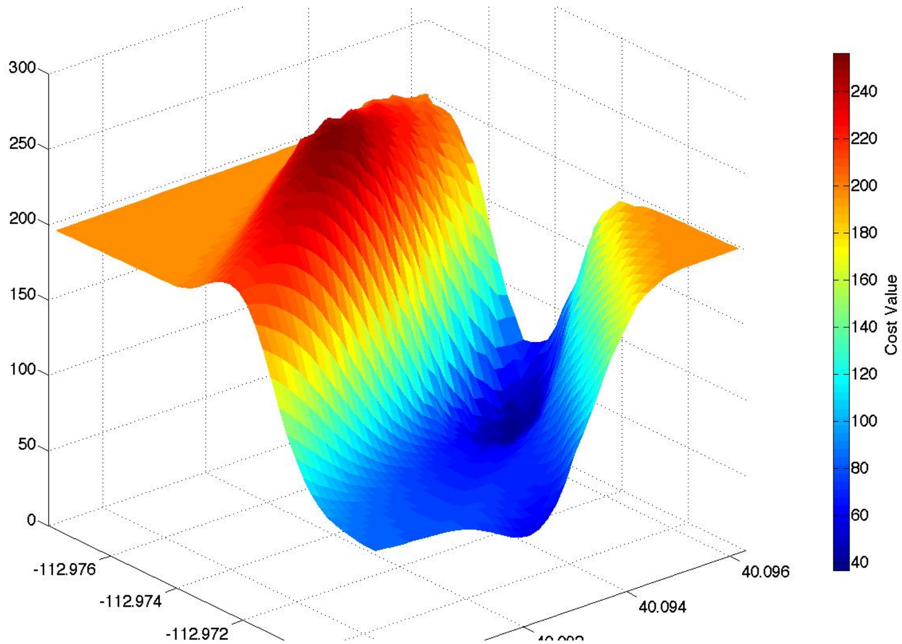
$$\sigma_{yy} = \sigma_{xx} \sin\left(\frac{\sigma_{\theta\theta}}{2}\right)$$

$$E_B = \begin{bmatrix} \sigma_{UU} \times \sigma_{tt} & 0 & 0 & 0 \\ 0 & \left[\left(\sigma_{UU} \times \sigma_{tt}\right) \times \sigma_{xx} \sin\left(\frac{\sigma_{\theta\theta}}{2}\right)\right]^2 & 0 & 0 \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \sigma_s^2 \end{bmatrix}$$

Leveraged 3 Uncertainties to Bind 2 Variables

Cost Function Comparison

Unconstrained Minimization



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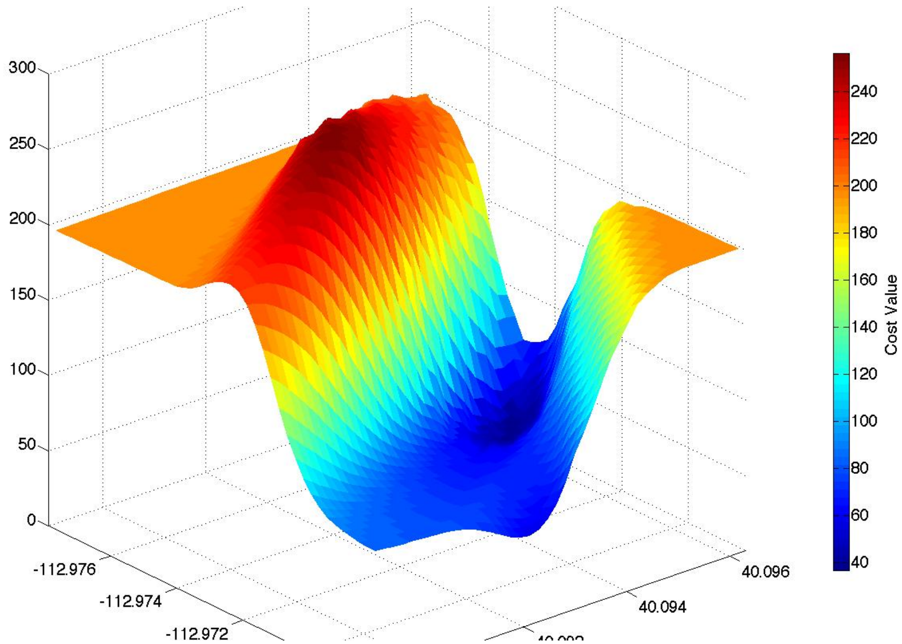
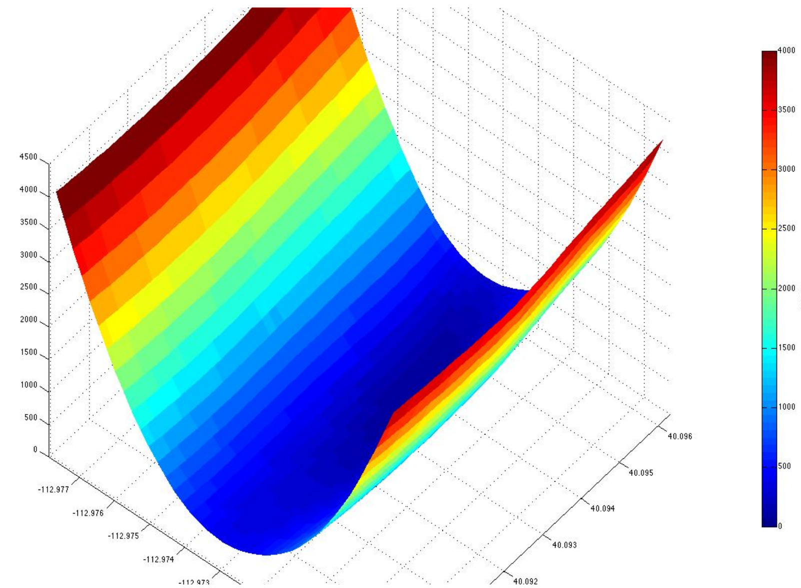


Constrained Minimization By Location (x_p, y_p)



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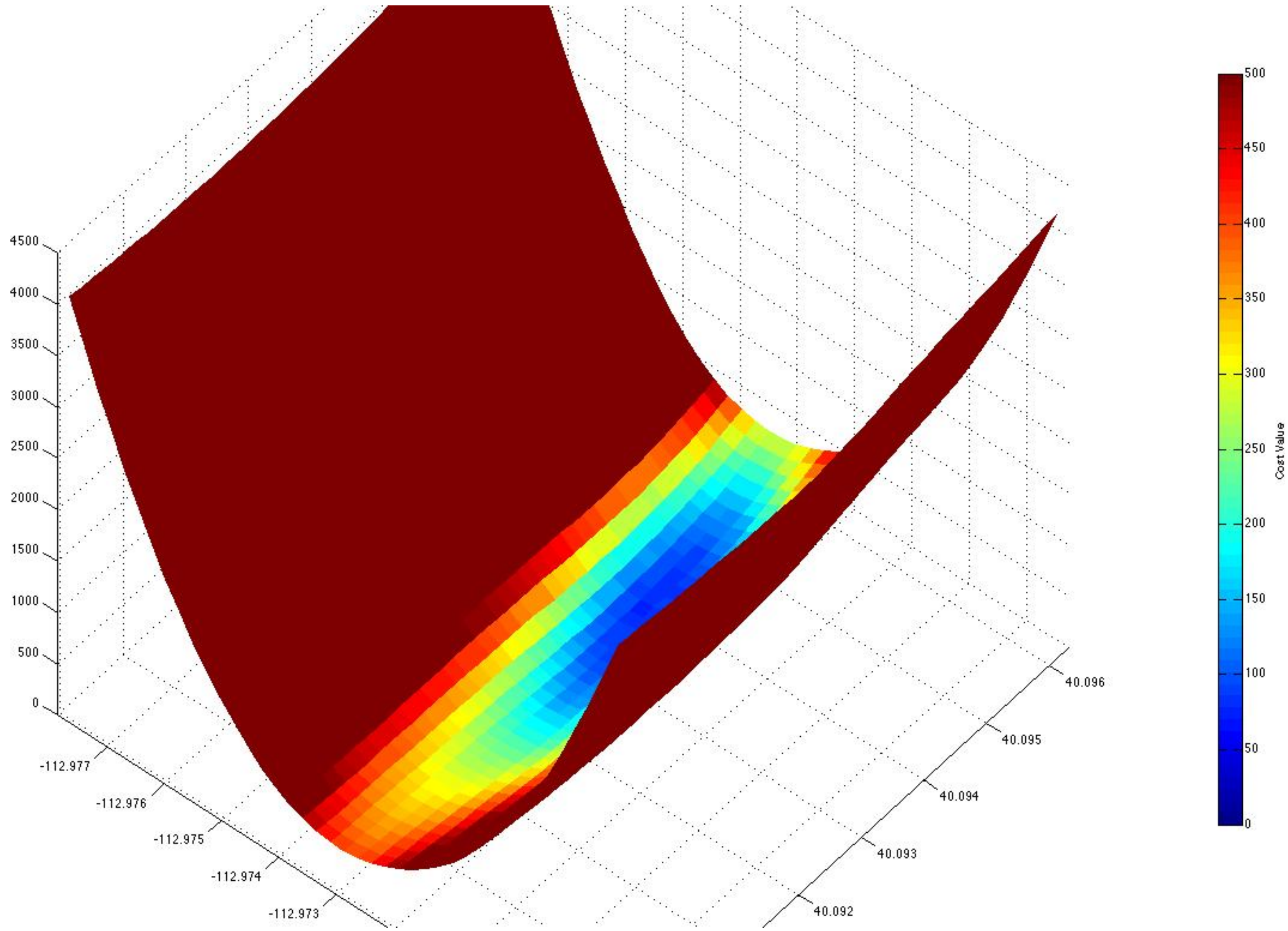

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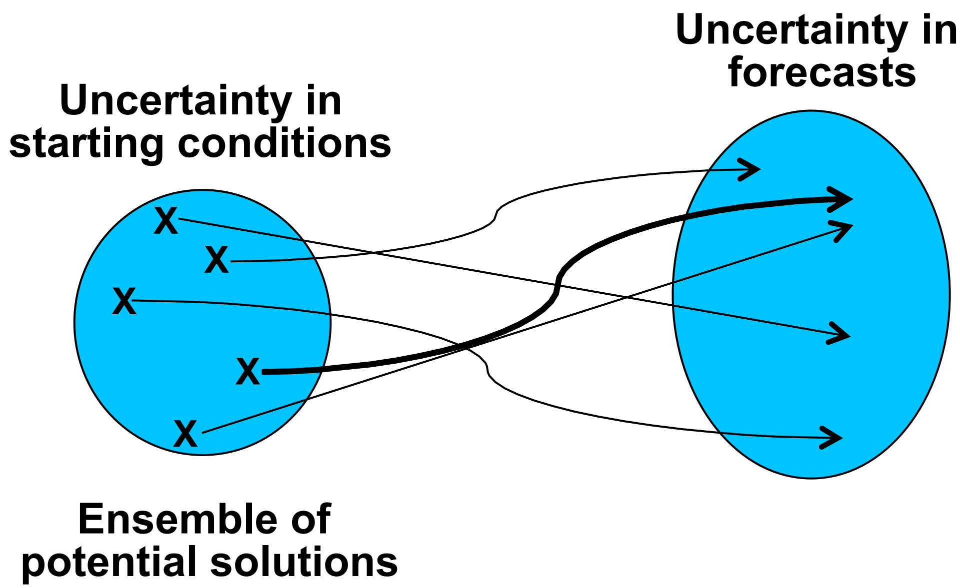
Background Error Covariance Matrix
(Mapping Uncertainty Directly Via Adjoint)

Standard ensemble



Run forward model

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Background Error Covariance Matrix

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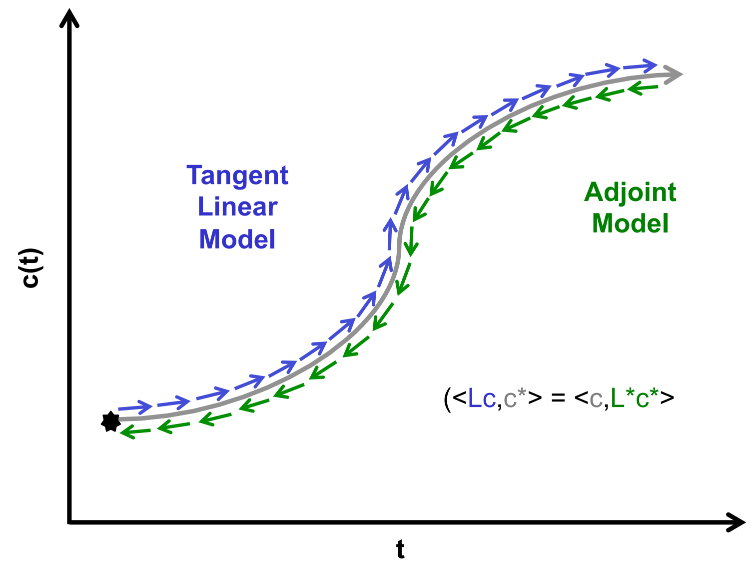
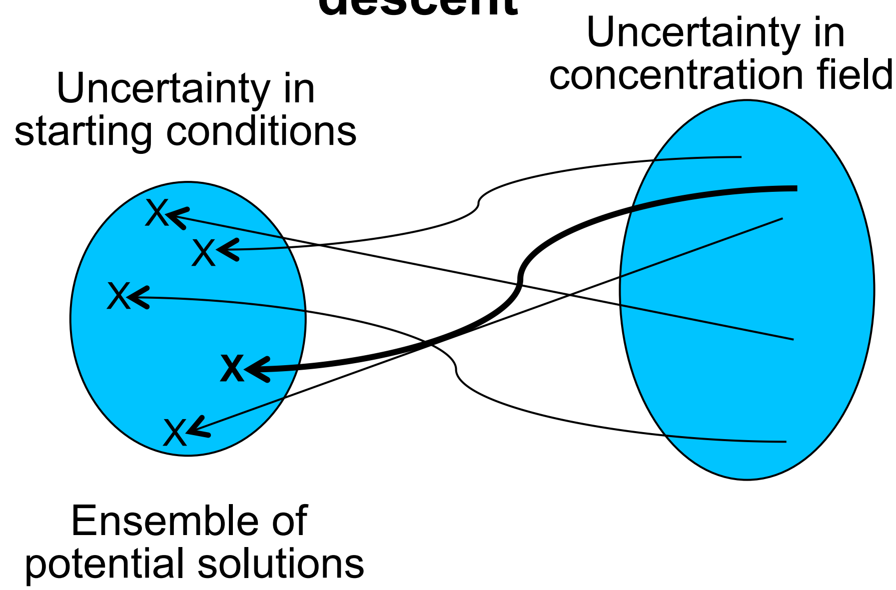


Ensemble by adjoint with gradient descent



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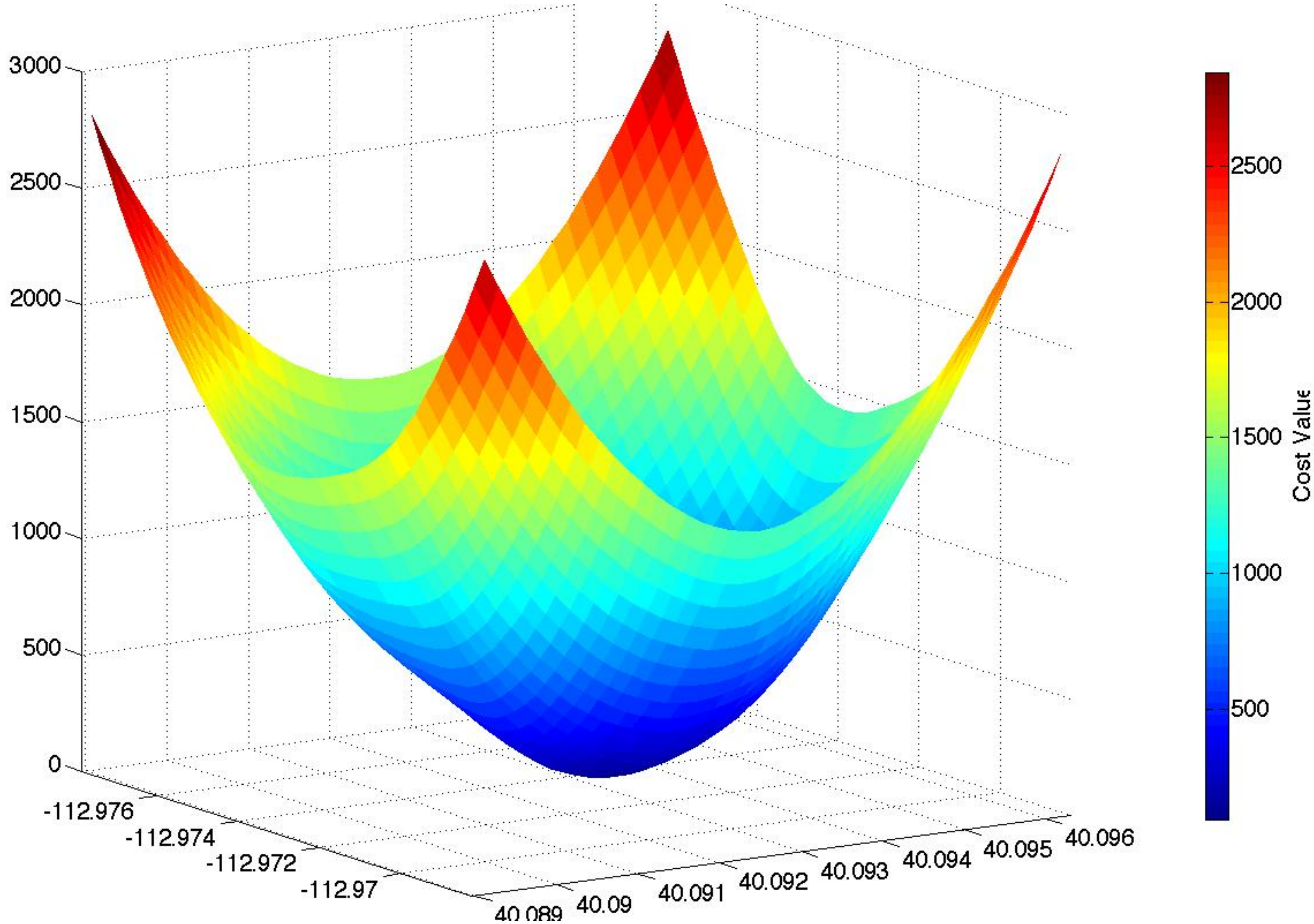
Conclusion


3000
2500
2000
1500
1000
500
0
-112.976
-112.974
-112.972
-112.97
40.089
40.09
40.091
40.092
40.093
40.094
40.095
40.096
2500
2000
1500
1000
500
Cost Value